AB INITIO STUDY OF ION-PAIR STATES OF THE IODINE MOLECULE

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Ion-pair states of the I_2molecule have been the subject of many experimentals studies and to date all 18 states correlating with $I^+(^3P_{J=2,1,0},\ ^1D_2) + I^-(^1S_0)$ asymptotes are known from experiment. This contribution reports on *ab initio* study of the I_2 molecule with an emphasis on the ion-pair states. Figure shows experimental and calculated potentials of the ion-pair states correlating with $I^+(^3P_2) + I^-(^1S_0)$ asymptote (energy is relative to I $(^2P_{3/2})$ + I $(^2P_{3/2})$ asymptote).